NIST Database for Simulation of Electron Spectra for Surface Analysis (SESSA)

(Standard Reference Database 100)

Version 1.0 of this database has been designed to facilitate quantitative interpretation of AES and XPS spectra and to improve the accuracy of quantitation in routine analysis. SESSA contains physical data needed to perform quantitative interpretation of an electron spectrum for a specimen of given composition. Retrieval of relevant data is performed by a small expert system [1-3] that queries the comprehensive databases. A simulation module provides an estimate of peak intensities as well as the energy and angular distributions of the emitted electron flux.

SESSA can be used for two main applications. First, data are provided for many parameters needed in quantitative AES and XPS (differential inverse inelastic mean free paths, total inelastic mean free paths, differential elastic-scattering cross sections, total elastic-scattering cross sections, transport cross sections, photoionization cross sections, photoionization asymmetry parameters, electron-impact ionization cross sections, photoelectron lineshapes, Auger-electron lineshapes, fluorescence yields, and Auger-electron backscattering factors). Second, Auger-electron and photoelectron spectra can be simulated for layered samples. The simulated spectra, for layer compositions and thicknesses specified by the user, can be compared with measured spectra. The layer compositions and thicknesses can then be adjusted to find maximum consistency between simulated and measured spectra. The design of the software allows the user to enter the required information in a reasonably simple way. The modular structure of the user interface closely matches that of the usual control units on a real instrument. In other words, any user who is familiar with a typical electron spectrometer can perform a retrieval/simulation operation with the SESSA software in a few minutes for a specimen with a given composition. Additional information on SESSA and some examples of SESSA applications are given at http://www.iap.tuwien.ac.at/%7Ewerner/sessa.html.

System requirements: PC with Windows operating system, CD-ROM drive, and a hard disc space of approximately 180 MB. The minimum amount of RAM needed to run SESSA is about 15 MB, but 30 MB or more is needed for simulations. SESSA is also available for Macintosh OS X and Linux operating systems, but these versions have not been as extensively tested as the Windows version.

Price: $1390 for a single copy (an order form is available on the NIST web site below). SESSA can be obtained for a free 15-day trial period at http://www.iap.tuwien.ac.at/~werner/asessa_demo.html.

Standard Reference Data Program
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1. W. Smekal, W. S. M. Werner, and C. J. Powell, Surf. Interface Anal. **37**, 1059 (2005).
2. W. S. M. Werner, Surf. Interface Anal. **31**, 141 (2001).
3. W. S. M. Werner, in *Surface Analysis by Auger and X-ray Photoelectron Spectroscopy*, D. Briggs and J. T. Grant, eds. (IMPublications, Chichester, 2003), p. 235.